Reduced effect of impurities on the universal pairing scale in the cuprates

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We consider the effect of non-magnetic impurities on the onset temperature T^* for the $d-$wave pairing in spin-fluctuation scenario for the cuprates. We analyze intermediate coupling regime when the magnetic correlation length $\xi/a > 1$ and the dimensionless coupling u is $O(1)$. In the clean limit, $T^* \approx 0.02 v_f/a$ in this parameter range, and weakly depends on ξ and u. We found numerically that this universal pairing scale is also quite robust with respect to impurities: the scattering rate Γ_{cr} needed to bring T^* down to zero is about 4 times larger than in weak coupling, in good quantitative agreement with experiments. We provide analytical reasoning for this result.

Introduction. The issue of the pairing glue in the cuprates is still one of the hottest topics in the physics of strongly correlated electrons. Many researchers believe that the pairing glue is a spin fluctuation exchange, at least in the overdoped and optimally doped cuprates. At such dopings correlations are relatively strong, but not enough so to break a large normal state Fermi surface (FS) into the hole and electron pockets.

Recently, Abanov *et al.* analyzed the pairing problem in the cuprates within spin-fluctuation scenario, under the assumption that the FS in the normal state is large.[1] Within this scenario, the onset of the pairing at $T = T^*$ marks the development of the pseudogap phase with strong thermal fluctuations of the pairing gap, and the true superconductivity emerges at a smaller $T_c \leq T^*$, when thermal fluctuations become weaker. These authors found a smooth crossover between the limit when the interaction U is smaller than v_f/a, and the pairing is confined to a vicinity of hot spots (points on the FS separated by (π, π)), and the limit of strong interaction, when the entire FS is "hot" (v_f is the bare Fermi velocity as obtained in band theory, and a is the interatomic spacing, $v_f/a \sim 1eV$). The onset temperature for the pairing, T^*, scales as $T^* \sim (v_f/a)u$ for $u = 3Ua/8\pi v_f \ll 1$, and as $T^* \sim (v_f/a)(1/u)$ at large u, and weakly depends on ξ for $\xi > a$. For intermediate values of $u = O(1)$, which are mostly relevant to the cuprates, T^* goes through a shallow maximum and is approximately $0.02 v_f/a$. The same pairing scale was obtained in FLEX calculations for the Hubbard model[2], in two-particle self-consistent calculations[3], in dynamical cluster approximation[4], and in cluster DMFT[5]. The good agreement between all these results is strong indication that $T^* \sim 0.02 v_f/a \sim 200 - 250K$ is indeed the universal pairing scale in optimally doped cuprates. At smaller dopings, this scenario breaks down because of electron localization which gives rise to precursors to hole and electron FS pockets already in the normal state. The pseudogap temperature T^* then becomes a scale at which the system develops such precursors, while the pairing emerges at a smaller temperature due to interaction between electron pockets.

The subject of this communication is the analysis of how the universal pairing scale T^* in optimally-doped cuprates is affected by non-magnetic impurities, which are pair-breaking for unconventional superconductors. In near-optimally doped cuprates, concentrations of dopants are quite substantial, and potential random scattering off dopants could significantly reduce T^*. At weak-coupling, which in our case corresponds to small u *and* $\xi \sim a$, non-magnetic impurities in a $d-$wave superconductor suppress T^* in the same way as magnetic impurities in a BCS superconductor, and T^* is given by Abrikosov-Gorkov (AG) formula [6] $\log T_0^*/T^* = \Psi(1/2 + \Gamma/2\pi T^*) - \Psi(1/2)$, (with $\Gamma/2$ instead of Γ for an s-wave and magnetic impurities[7]), where $\Psi(x)$ is the di-Gamma function and T_0^* is the pairing temperature in the absence of impurities. The ratio of the critical value of the scattering, $\Gamma_{cr} : T^*(\Gamma_{cr}) = 0$, to T_0^* is $\Gamma_{cr}/T_0^* = \pi/2e^{0.5772} \approx 0.88$.

The issue we address here both analytically and numerically is what is this ratio when $u = O(1)$ and $\xi \gg a$, when the pairing problem involves incoherent fermions and near-gapless dynamical bosons and is very different from the $d-$wave version of the BCS theory. We find that in this situation the ratio Γ_{cr}/T_0^* is about 4 times larger than 0.88, i.e., the pairing is much less suppressed by impurities than in the weak coupling. This result is in agreement with the experiments which observed[8] a similar reduction of the slope of $T^*(\Gamma)$ compared with the AG formula.

Another issue that we consider here is how impurity scattering affects the angular dependence of the $d-$wave pairing gap. For a clean system, Abanov *et al.* have found[1] that in the universal regime the form of the gap $\Delta_p(\omega)$ is very close to $\cos p_x - \cos p_y$ for all frequencies. We show that the $\cos p_x - \cos p_y$ form holds in the presence of impurities – the angular dependence only slightly changes with Γ. The implication is that both T^* and the gap structure are robust towards impurities.

The angular dependence of the gap, particularly in underdoped cuprates, has been the subject of intensive debates recently, and some ARPES data were interpreted as evidence for strong deviations from the $\cos p_x - \cos p_y$ form. We emphasize in this regard that the position of the maximum of the spectral function $A_p(\omega)$ represents

the pairing gap $\Delta_p(\omega)$ only deep in the superconducting state. At higher T, the position of the maximum in $A_p(\omega)$ differs from $\Delta_p(\omega)$ because of damping induced by scattering off thermal bosons. In particular, even for a gap with a perfect $\cos p_x - \cos p_y$ form a maximum in $A_p(\omega = 0)$ is still present in some neighborhood of a node (a Fermi arc). In this regard, our result that the gap keeps $\cos p_x - \cos p_y$ form even in the presence of impurities agrees with ARPES data by Campuzano *et al.*,[9] who detected this form at the lowest T.

The effects of non-magnetic and magnetic impurities in superconductors with unconventional order parameters have been studied for high-T_c cuprates,[10,11,12,13,14,15] non-cuprate superconductors,[16,17,18,19] and most recently for the pnictides.[20,21] For the cuprates, most of the studies attributed a slow decrease of T^* to the extended nature of the impurity potential[12,13,14], but Monthoux and Pines[10] performed a numerical analysis of T^* suppression in YBCO by non-magnetic Ni impurities and found that the initial slope of T^* is quite small even when impurities are point-like scatterers. Very recently, Kemper *et al.*[15] studied the effect of disorder using dynamical cluster approximation and quantum Monte Carlo, and found that ordinary pair-breaking by impurities is partly balanced by the impurity-induced enhancement of spin correlations which increases the pairing interaction mediated by spin fluctuations

Our result agree with Kemper *et al.*[15] and also Graser *et al.*[14] in that the origin of the flattening of $T^*(\Gamma)$ are magnetic strong-correlation effects. At the same time, we found that, in the universal regime, T^* very weakly depends on the spin correlation length ξ. In our theory, softness of T^* suppression compared to weak-coupling AG theory is primarily associated with the strong frequency dependence of the pairing interaction.

Theory. We follow earlier work[1] and consider fermions with a large FS and $d-$wave pairing mediated by overdamped spin fluctuations. We add to earlier analysis an isotropic, elastic scattering by point-like impurities. As customary for the pairing problem, we introduce normal and anomalous Green's functions and self-energies and treat spin-fluctuation mediated pairing within the Eliashberg theory, by keeping self-energies but neglecting vertex corrections. For small and large u's, this approximation can be rigorously justified because vertex corrections are small in u or $1/u$, respectively. For $u = O(1)$, it can only be justified on the basis that vertex corrections are small numerically.[22]

The set of equations includes fermionic and bosonic self-energies in the normal state, and the linearized equation for the $d-$wave pairing vertex $\Phi^{\chi}_{\boldsymbol{p}_f}(\omega_m)$ (Ref.1)

$$\Sigma_{\boldsymbol{p}_f}(\omega_m) = \pi T^* \sum_{\omega'_m} \int d\boldsymbol{p}'_f \chi^{\omega_m-\omega'_m}_{\boldsymbol{p}_f-\boldsymbol{p}'_f} \,\mathrm{sign}(\omega_m\omega'_m)\,, \quad (1)$$

$$\Phi^{\chi}_{\boldsymbol{p}_f}(\omega_m) = -\pi T^* \sum_{\omega'_m} \int d\boldsymbol{p}'_f \frac{\chi^{\omega_m-\omega'_m}_{\boldsymbol{p}_f-\boldsymbol{p}'_f}\Phi_{\boldsymbol{p}'_f}(\omega'_m)}{|\omega'_m| + \Gamma + \Sigma_{\boldsymbol{p}'_f}(\omega'_m)}\,, \quad (2)$$

$$\Phi_{\boldsymbol{p}_f}(\omega_m) = \Phi^{\chi}_{\boldsymbol{p}_f}(\omega_m) + \Gamma \int \frac{d\boldsymbol{p}'_f\ \Phi_{\boldsymbol{p}'_f}(\omega_m)}{|\omega_m| + \Gamma + \Sigma_{\boldsymbol{p}'_f}(\omega_m)}\,, \quad (3)$$

$$\chi^{\Delta\omega}_{\boldsymbol{p}_f-\boldsymbol{p}'_f} = \frac{(ua/\pi)}{(a/\xi)^2 + a^2|\boldsymbol{p}_f - \boldsymbol{p}'_f - \boldsymbol{Q}|^2 + |\Delta\omega|/\Omega}\,, \quad (4)$$

where $\Omega = 3v_f/(16ua)$ and momenta $\boldsymbol{p}_f$ in all formulas are confined to the FS, because integration in the direction transverse to the FS has been carried out. In distinction to Ref. 1 in (2), (3) we also included impurity renormalization of $\Phi^{\chi}_{\boldsymbol{p}_f}$, and of Matsubara energies $\omega_m = \pi T^*(2m+1)$, where $\Gamma = (n_i/\pi N_f)\sin^2\delta$ depends on impurity concentration n_i, fermionic density of states N_f, and the impurity potential u_0 via $\tan\delta = \pi u_0 N_f$.

The set of equations for Φ and Σ can be simplified in the usual way by introducing mass renormalization factor $Z_{\boldsymbol{p}_f}(\omega_m)$ and the pairing gap $\Delta_{\boldsymbol{p}_f}(\omega_m)$ via

$$Z_{\boldsymbol{p}_f}(\omega_m) = \frac{|\omega_m| + \Gamma + \Sigma_{\boldsymbol{p}_f}(\omega_m)}{|\omega_m|}\,, \quad \Delta_{\boldsymbol{p}_f}(\omega_m) = \frac{\Phi_{\boldsymbol{p}_f}(\omega_m)}{Z_{\boldsymbol{p}_f}(\omega_m)}\,. \quad (5)$$

Due to A_{1g} symmetry of $\Sigma_{\boldsymbol{p}_f}$ and B_{1g} symmetry of $\Phi^{\chi}_{\boldsymbol{p}_f}$ the impurity renormalization of the pairing vertex vanishes, i.e., $\Phi_{\boldsymbol{p}_f} = \Phi^{\chi}_{\boldsymbol{p}_f}$. Using (5) we obtain from (2)

$$\sum_{\omega'_m} \int d\boldsymbol{p}'_f \left[\pi T \frac{\chi^{\omega_m-\omega'_m}_{\boldsymbol{p}_f-\boldsymbol{p}'_f}}{|\omega'_m||\omega_m|} + \delta_{mm'}\delta_{\boldsymbol{p}_f\boldsymbol{p}'_f}\ \frac{Z(\omega_m,\boldsymbol{p}_f)}{|\omega_m|}\right]\Delta(\omega'_m,\boldsymbol{p}'_f) = 0. \quad (6)$$

We wrote the gap equation as an eigenvalue problem by moving all terms to one side and symmetrizing the kernel with respect to $\omega_m, \omega_{m'}$.

Numerical solution. This linearized gap equation is solved numerically by presenting the FS integral as a sum, varying T and finding T^* as the highest temperature where Eq. (6) is satisfied. The result is presented in Fig. 1. We clearly see a strong increase of the ratio Γ_{cr}/T^*_0 compared with a BCS $d-$wave superconductor. For $u \sim 1$, when T^*_0 as a function of u has a maximum at about $0.02v_f/a$, this ratio is nearly 4 times larger than in the BCS limit. This result is in a good *quantitative*

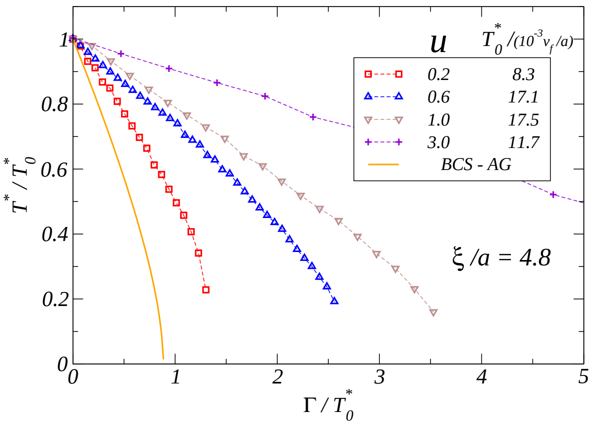

FIG. 1: (Color online) The onset temperature for the pairing, T^*, vs. Γ for different values of u. T_0^* is the pairing temperature in the clean limit. $v_f/a \sim 1eV$ in the cuprates, hence $10^{-3}v_f/a \simeq 1\,meV$. We set $\xi/a = 4.8$ for definiteness. The solid line is AG-type result for a BCS $d-$wave superconductor, which in our case corresponds to the limit $u\xi \ll 1$. The key result in this figure is a progressive increase with u of the critical ratio Γ_{cr}/T_0^*, at which $T^* = 0$. For $u = O(1)$, this ratio is about 4 times larger than in the BCS limit. The transition temperature is found with relative precision 10^{-2}. The range of low T requires special care because for any finite number of Matsubara points the curve $T^*(\Gamma)$ bends back towards the origin producing a spurious second solution.

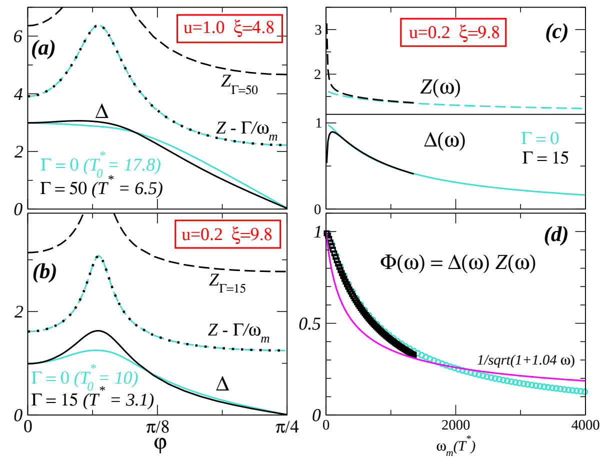

FIG. 2: (Color online) Left: the angular dependence of the quasiparticle renormalization factor $Z_{\boldsymbol{p}_f}(\omega_{m=0})$ and of the gap function $\Delta_{\boldsymbol{p}_f}(\omega_0)$ for $u = 1$, $\xi = 4.8a$ (a) and $u = 0.2$, $\xi = 9.8a$ (b). T^*, Γ and ω_m are in units of $10^{-3}v_f/a$. Observe that the angular dependences of the gap and Z (with subtracted constant shift due to Γ) changes very little between $\Gamma = 0$(light lines) and $\Gamma \lesssim \Gamma_{cr}$(dark lines). Panel (c): frequency dependences of $\varphi = 0$ $\Delta_{\boldsymbol{p}_f}(\omega_m)$ and $Z_{\boldsymbol{p}_f}(\omega_m)$. Panel (d): the comparison of the numerically obtained frequency dependence of $\Phi_{\varphi=0}(\omega_m)$ with the analytic solution of Eq. (7) in which momentum dependence of the gap near hot spot is neglected.

agreement with the experiment in Ref. 8 and shows that the universal pairing scale in the cuprates is resistant to ordinary impurities.

In Fig. 2 on the left we show the angular dependences of the quasiparticle renormalization factor $Z_{\boldsymbol{p}_f}(\omega_0) = 1 + [\Sigma_{\boldsymbol{p}_f}(\omega_0) + \Gamma]/\omega_0$ and of the gap function $\Delta_{\boldsymbol{p}_f}(\omega_0)$ for clean and dirty cases, for $\omega_0 = \pi T^*$ and different u and ξ. In the clean case and $u = O(1)$ the angular dependence is quite close to $\cos 2\phi$ (or $\cos p_x - \cos p_y$). We see that the effect of the impurities on the angular dependence of the gap is quite small, i.e., $\cos 2\phi$ form is preserved in a dirty case. We verified that this holds for all Γ up to the critical value, and for all Matsubara frequencies. For completeness, in Fig. 2(c) we show the frequency dependences of $Z_{\boldsymbol{p}_f}(\omega_m)$ and $\Delta_{\boldsymbol{p}_f}(\omega_m)$, and in panel (d) we present $\Phi_{\boldsymbol{p}_f}(\omega_m)$ at $\varphi = 0$ which we will later compare with the analytical formula.

Analytical reasoning. To understand the origin of the increase of Γ_{cr}/T_0^* we analyze the equation for the pairing vertex $\Phi_{\boldsymbol{p}_f}(\omega_m)$ analytically at $T = 0$, i.e., we look for a solution near Γ_{cr}. To do this, we make an approximation and neglect angular dependence of the gap near a hot spot. The momentum integration along the FS then can be carried out analytically, and the equation for the gap at a hot spot becomes 1D integral equation in frequency only. This equation is more easy to analyze than the original $3D$ integral equation. The approximation of the gap function by a constant near hot spots can be rigorously justified at small u (corrections are higher powers of u), but remains qualitatively valid up to $u = O(1)$ (Ref. 1).

The expression for T_0^* in this approximation has been obtained earlier[23] – $T_0^* \approx 0.13u(v_f/a)$, with very weak dependence on ξ as long as $u\xi > 1$. For small $u\xi$, T_0^* is described by a BCS formula.

Using $\Phi_{\boldsymbol{p}_f+\boldsymbol{Q}}(\omega_m) = -\Phi_{\boldsymbol{p}_f}(\omega_m)$, dropping the dependence of $\boldsymbol{p}_f$ near a hot spot, integrating over momentum in Eqs. (1) - (3), and rescaling variables, we obtain after some algebra the equation for $\Phi(\omega_m)$ at $T = 0$ in the form

$$\Phi(x) = \frac{\lambda}{2}\int_0^\infty dy \frac{\Phi(y)}{y + \tilde{\Gamma} + \frac{2\lambda y}{1+\sqrt{4\lambda^2 y+1}}} \times \left(\frac{1}{\sqrt{4\lambda^2|y-x|+1}} + \frac{1}{\sqrt{4\lambda^2|y+x|+1}}\right), \quad (7)$$

where x, y are frequencies in units of $\bar{\omega} = (3u/4)v_f/a$, $\tilde{\Gamma} = \Gamma_{cr}/\bar{\omega}$, and $\lambda = (2u\xi)$ (mass renormalization in the normal state is $1 + \lambda$).

Weak coupling BCS limit corresponds to $\lambda \ll 1$. In this limit, $\Phi(x)$ becomes independent of x (and $\Phi = \Delta$), the gap equation is solved in the same way as in AG theory, and the value of $\Gamma_{cr}/T_0^* \approx 0.88$. We, however, are interested in the opposite limit, when $\lambda > 1$. We analyzed equation (7) by normalizing $\Phi(x)$ to $\Phi(0) = 1$, expanding at small x and at large x and extrapolating between the two limits. At small x, $\Phi = 1 - O(x)$, at large x, $\Phi(x) \propto 1/\sqrt{x}$. We found that $\Phi(x)$ is well approximated by $\Phi(x) = 1/\sqrt{1+cx}$, where c is a constant which depends on λ and $\tilde{\Gamma}$. The error is less than 2% for all x

and for all λ which we considered. We also checked that that this solution is not an artefact: if we use this $\Phi(x)$ as an input and run iterations, $\Phi(x)$ rapidly converges. The critical value of $\tilde{\Gamma}$ is then obtained by substituting this form back into (7) and solving for $\Phi(0) = 1$.

Carrying out this procedure, we found that *c increases* with increasing $\lambda = u\xi$, i.e., when the correlation length increases and the pairing problem becomes more and more non-BCS, the gap function gets confined to progressively smaller frequencies. The $c(\lambda)$ increases from $c(1) = 0.66$, through $c(2) = 1.04$ and $c(5) = 1.7$, to $c(\infty) = 2.31$. In Fig. 2(d) we compare our approximate analytic $\Phi(\omega_m)$ for $u = 0.2$, $\xi = 9.8a$ ($\lambda \approx 2$) with the numerical $\Phi_{\boldsymbol{p}_f}(\omega_m)$. We see that the agreement is expectedly not prefect, but generic trends of the frequency dependence is captured by the approximate solution.

Substituting $\Phi(x) = 1/\sqrt{1 + cx}$ back into (7) and solving for $\Phi(0) = 1$, we found that $\tilde{\Gamma}$ progressively increases as λ gets larger, from $\lambda^{-2}e^{-1/\lambda}$ at small λ to 0.3 for $\lambda = 1$ and to 0.46 for $\lambda = \infty$.

The monotonic increase of the value of $\tilde{\Gamma}$ with increasing λ is a tricky effect. One could expect that the confinement of $\Phi(x)$ to smaller x as λ increases and the increase of the self-energy tend to reduce $\tilde{\Gamma}$ simply because typical frequencies get smaller. However, as λ increases, the interaction strength also increases, and this tends to increase $\tilde{\Gamma}$ because $\tilde{\Gamma}$ appears in the denominator in the integral for $\Phi(0) = 1$, and larger $\tilde{\Gamma}$ are required to balance the increase of the interaction. We compared the two effects and found that increase of the interaction overshadows other effects and is the origin of the growth of $\tilde{\Gamma}$ with increasing λ.

We next compared the growth of $\Gamma_{cr} = \bar{\omega}\tilde{\Gamma}(\lambda)$ and the grown of T^*_0. The latter also scales as $\bar{\omega}$ with λ-dependent prefactor (Ref. 23). This prefactor increases with increasing λ, but its λ-dependence is very weak: it changes by less than 5% between $\lambda = 1$ and $\lambda = \infty$. As a result, the λ-dependence of the ratio Γ_{cr}/T^*_0 predominantly comes from $\tilde{\Gamma}(\lambda)$, which, we remind, increases with λ. Inserting the numbers, we find that the ratio Γ_{cr}/T^*_0 becomes 2.0 for $\lambda = 1$; 2.37 for $\lambda = 2$; 2.47 for $\lambda = 5$, and 2.74 for $\lambda = \infty$. The scale of the increase is quite consistent with what we found numerically in Fig. 1 by solving the full 3D integral equation in momentum and frequency.

Summary. In this paper we considered the effect of non-magnetic impurities on the onset temperature T^* for the $d-$wave pairing in spin-fluctuation scenario for the cuprates. Non-magnetic impurities are pair-breaking for $d-$wave superconductivity, and one should expect a reduction of T^* due to impurities. In weak-coupling, T^* falls off rapidly, following the AG curve.

We analyzed the effect of impurities in the intermediate coupling regime when the magnetic correlation length $\xi/a > 1$, the dimensionless coupling u is $O(1)$, and the pairing problem is qualitatively different from BCS. In the clean limit, T^* in this parameter range weakly depends on ξ and u and is approximately $0.02v_f/a$. We found that this universal pairing scale is quite robust with respect to impurities: the critical value of the scattering rate Γ_{cr} needed to bring T^* down to zero is about 4 times larger than in the weak coupling. This implies that the slope of the initial reduction of T^* is weaker by about the same factor than in the weak coupling. This reduction of the slope agrees with the experiments[8] and with earlier work by Monthoux and Pines[10] on T^* suppression in YBCO due to non-magnetic Ni impurities. We also analyzed the angular dependence of the gap and found that it is little affected by impurities.

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